Question 1

We consider the following reaction in gas phase.

A + 3B⇔2C

At first, A and B exist in the stoichiometic ratio, and there is no C in the reaction system. Now, we think ξ is "extent of reaction" or "progress variable". Describe ξ by using total pressure of this reaction gas mixture system, p0. K is a equilibrium constant of this reaction and independent of the pressure.

Answer 1

	A	+	3B	↔	2C
t=0	n		3n		0
t	n-x		3n-3x		2x
t=tf	n-ξ		3n-3ξ		2ξ

$$K = \prod_{i=1}^{N} \alpha_i(f)^{\nu_i}$$

Where α is the activity and ν the stoichiometric coefficient

$$K = \alpha_a(f)^{\nu_a} * \alpha_b(f)^{\nu_b} * \alpha_c(f)^{\nu_c}$$

$$K = \frac{\alpha_c(f)^2}{\alpha_a(f) * \alpha_b(f)^3}$$

$$\alpha_i(f) = \frac{n_i}{n_{tot}} * \frac{p^0}{p_0}$$

Where p_0 is the reference pressure

$$K = \frac{(\frac{n_c}{n_{tot}} * \frac{p^0}{p_0})^2}{\frac{n_a}{n_{tot}} * \frac{p^0}{p_0} * (\frac{n_b}{n_{tot}} * \frac{p^0}{p_0})^3}$$

$$n_{tot} = n_a + n_b + n_c$$

$$n_{tot} = 4n - 2\xi$$

$$K = \frac{(\frac{3n - 3\xi}{4n - 2\xi} * \frac{p^0}{p_0})^2}{\frac{n - \xi}{4n - 2\xi} * \frac{p^0}{p_0} * (\frac{2\xi}{4n - 2\xi} * \frac{p^0}{p_0})^3}$$

$$K = \frac{(\frac{3n - 3\xi}{4n - 2\xi})^2}{\frac{n - \xi}{4n - 2\xi} * (\frac{2\xi}{4n - 2\xi})^3 * (\frac{p^0}{p_0})^2}$$

$$K = \frac{9 * (\mathrm{n} - \xi)^2 * 4 * (2n - \xi)^2}{8 * (\mathrm{n} - \xi) * (\xi)^3 * (\frac{p^0}{p_0})^2}$$

$$K = \frac{9 * (\mathrm{n} - \xi) * (2n - \xi)^2}{2 * (\xi)^3 * (\frac{p^0}{p_0})^2}$$

$$K = \frac{9 * (\mathrm{n} - \xi) * (2n - \xi)^2}{2 * (\xi)^3} (\frac{p_0}{p^0})^2$$

$$K = \frac{9 * (\mathrm{n} - \xi) * (4n^2 + \xi^2 - 4n\xi)}{2 * (\xi)^3} (\frac{p_0}{p^0})^2$$

$$K = \frac{9 * (4n^3 + n\xi^2 - 4n^2\xi + 4n^2\xi - \xi^3 + 4n\xi^2)}{2 * (\xi)^3} (\frac{p_0}{p^0})^2$$

$$K = \frac{9 * (4n^3 - \xi^3 + 5n\xi^2)}{2 * (\xi)^3} (\frac{p_0}{p^0})^2$$

$$2 * (\xi)^3 K = 9 * (4n^3 - \xi^3 + 5n\xi^2)(\frac{p_0}{p^0})^2$$

$$\left(2 * K - 9 * \left(\frac{p_0}{p^0}\right)^2\right)\xi^3 - 40 * n\left(\frac{p_0}{p^0}\right)^2 \xi^2 + 36 * n^3\left(\frac{p_0}{p^0}\right)^2 = 0$$

We need now to solve this equation